Two 2D spin crossover coordination polymers constructed by $[Pd(SCN)_4]^{2-}$ building blocks

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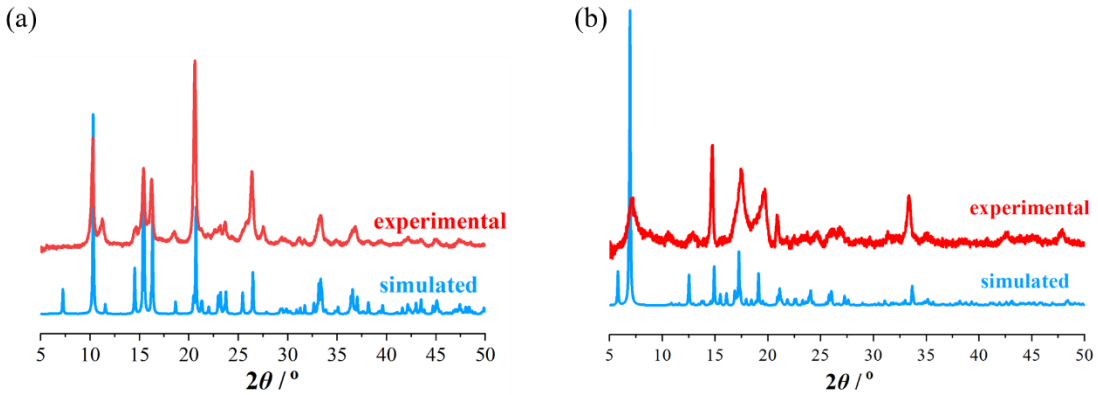

Figure S1. Powder X-ray diffraction data of **1** (a) and **2** (b).

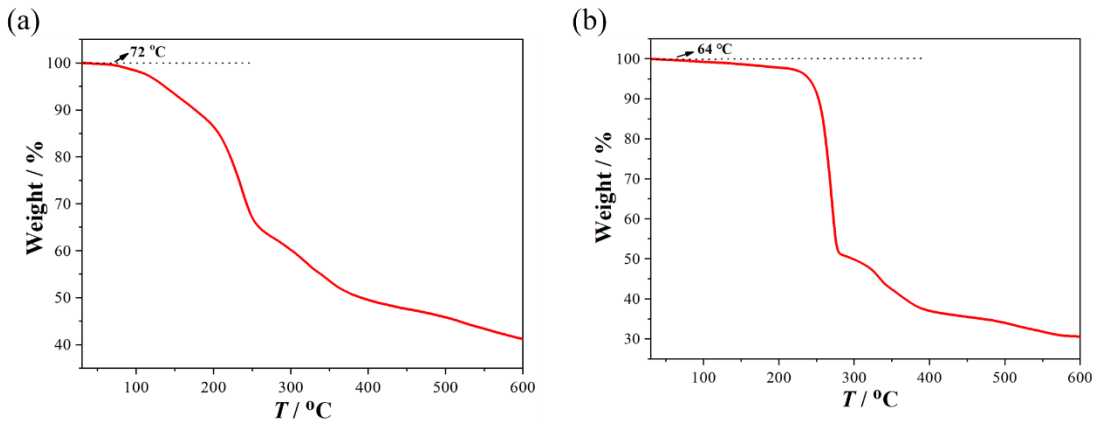

Figure S2. Thermogravimetric analyses of **1** (a) and **2** (b).

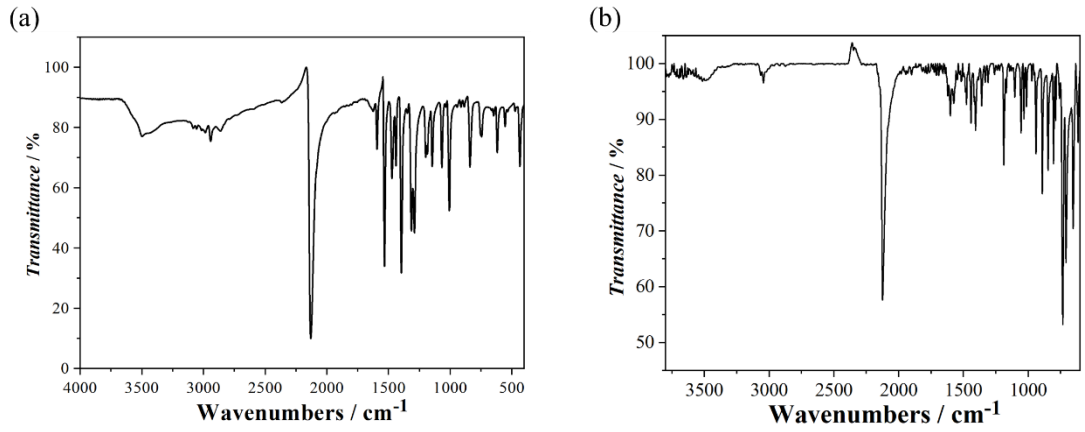

Figure S3. IR spectra of **1** (a) and **2** (b).

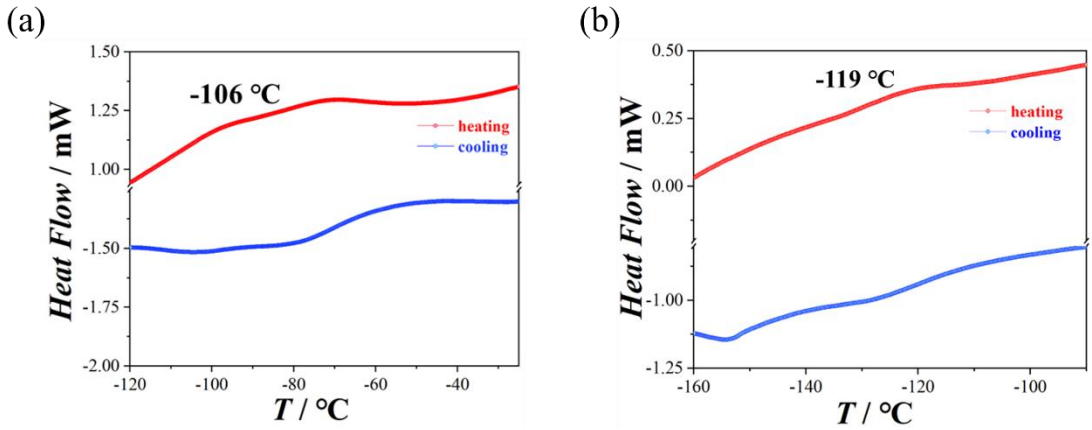

Figure S4. Differential scanning calorimetry (DSC) measurements of **1** (a) and **2** (b).

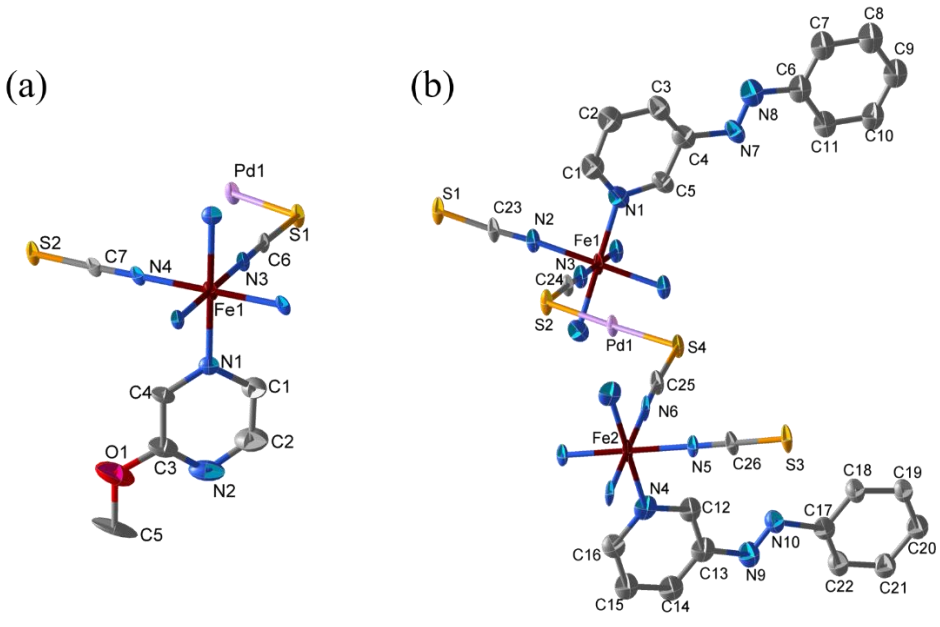

Figure S5. Asymmetric units of **1** (a) and **2** (b). Hydrogen atoms are omitted for clarity.

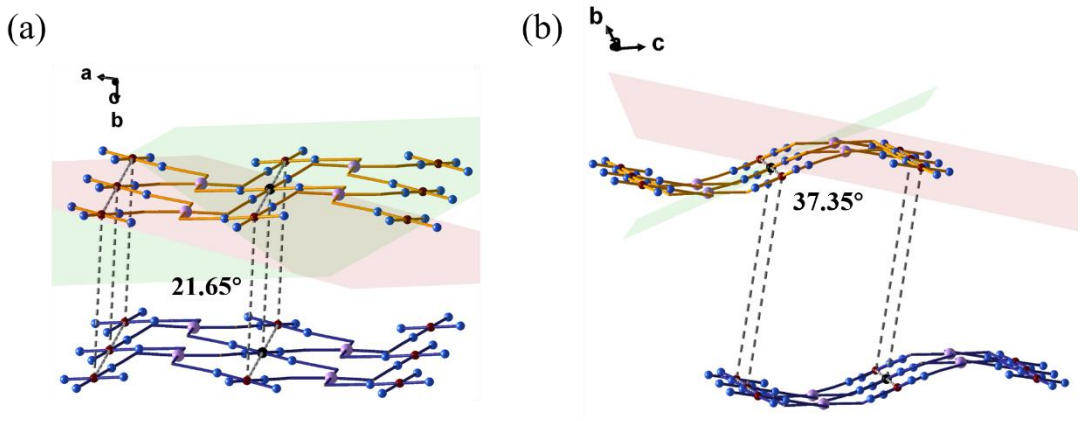

Figure S6. The dihedral angles of **1** (a) and **2** (b).

Table S1. Selected structural parameters for **1** and **2** at different temperatures.

	1		**2**	
Parameter	**100 K**	**245 K**	**110 K**	**200 K**
<Fe−N_{SCN}>	<Fe1–N3>1.931(1)	<Fe1–N3>2.126(1)	<Fe1–N2>1.947(4)	<Fe1–N2>2.134(4)
	<Fe1–N4>1.939(2)	<Fe1–N4>2.134(2)	<Fe1–N3>1.950(4)	<Fe1–N3>2.103(5)
			<Fe2–N5>1.937(4)	<Fe2–N5>2.119(4)
			<Fe2–N6>1.920(3)	<Fe2–N6>2.114(4)
<Fe−N_{py}>	<Fe1–N1>2.006(2)	<Fe1–N1>2.200(2)	<Fe1–N1>2.003(5)	<Fe1–N1>2.180(6)
			<Fe2–N4>2.004(5)	<Fe2–N4>2.177(5)

Table S2. The shortest Fe···Fe distance and dihedral angles of **1** and **2**.

	1		**2**	
Parameter	**100 K**	**245 K**	**110 K**	**200 K**
Fe···Fe[a]	8.398(8)	8.577(8)	8.284 (2)	8.448(2)
Fe···Fe[b]	9.407(7)	9.592(7)	13.302(3)	13.455(3)
Dihedral angles[c]	21.651	23.524	37.351	41.870
Dihedral angles[d]	14.986	15.410	26.325	26.891
Dihedral angles[e]	14.450	14.740	27.194	27.940

[a] The shortest Fe···Fe distance within the layer (Å); [b] The shortest Fe···Fe distance between layers (Å); [c] The dihedral angles between the two [FeN_4] faces (°); [d] The dihedral angles between the two Fe···Pd···Fe faces in the quadrilateral (°); [e] The dihedral angles between the two Fe···S−Pd−S···Fe faces in the quadrilateral (°).

Table S3. Ligand-ligand interaction between adjacent layers of **1**.

	1	
Parameter	**100 K**	**245 K**
Centroid[a]···Centroid[b]	4.548(4) Å	4.555(4) Å
O1[a]···N2[b]	3.752(2) Å	3.712(2) Å
O1[a]···O1[b]	4.199(4) Å	4.290(4) Å

N2^{a}···N2^{b}	4.322(4) Å	4.446(4) Å
N1^{a}···N2^{b}	4.719(4) Å	4.731(4) Å
N2^{a}···N1^{b}	4.416(3) Å	4.449(3) Å

Centroid: N1-N2, C1-C4; a: x, y, z; b: x, 1-y, -0.5+z.

Table S4. In-layer ligand-ligand interaction of **2**.

	2	
Parameter	**110 K**	**200 K**
N7^{a}···N9^{b}	3.598(2) Å	3.830(7) Å
N8^{a}···N9^{b}	3.654(8) Å	3.794(9) Å
N7^{a}···N10^{b}	3.778(8) Å	3.913(9) Å
N8^{a}···N10^{b}	4.189(1) Å	4.232(1) Å
N1^{a}···C18^{b}	3.899(7) Å	3.890(7) Å
N1^{a}···C17^{b}	4.224(6) Å	4.188(6) Å
N1^{a}···C19^{b}	4.266(9)	4.263(9)
C11^{a}···N4^{b}	3.892(8) Å	3.925(8) Å
C10^{a}···N4^{b}	4.194(1) Å	4.247(1) Å
C6^{a}···N4^{b}	4.371(8) Å	4.283(9) Å

a: x, y, z; b: 1-x, 1-y, 1-z.